

4,4'-[(1,3-¹³C₂)Propane-2,2-diyl]diphenol
263261-64-9 | DTXSID30747173

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 3.48

Global applicability domain: Inside

Local applicability domain index: 5.44e-01

Confidence level: 7.92e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-Cyclohexylphenylacetic acid</div> <div>Measured: 3.91</div> <div>Predicted: 3.90</div>	<div>Image not found</div> <div>Bisphenol A</div> <div>Measured: 3.32</div> <div>Predicted: 3.20</div>	<div>Image not found</div> <div>4-Hexylresorcinol</div> <div>Measured: 3.45</div> <div>Predicted: 3.66</div>
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